



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:17 AM UTC

PDB ID : 2BJY / pdb_00002bjy
Title : The X-ray crystal structure of Listeria innocua Dps H31G-H43G mutant.
Authors : Ilari, A.; Stefanini, S.; Chiancone, E.
Deposited on : 2005-02-08
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

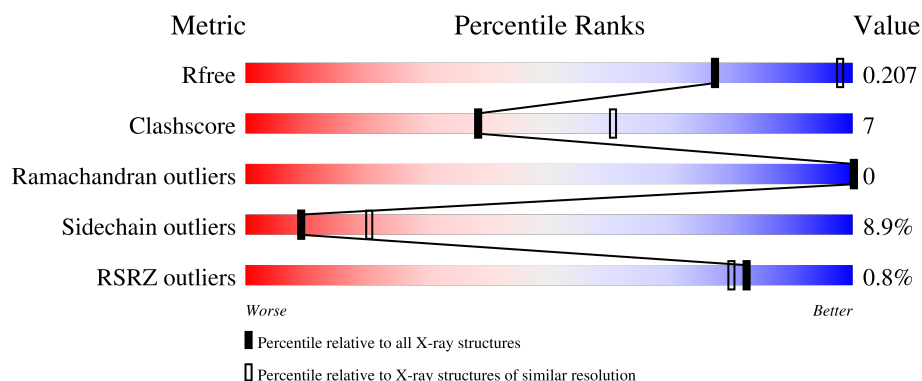
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



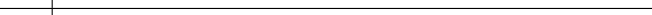
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	156	% 79% 13% ...
1	B	156	72% 22% ...
1	C	156	81% 12% ...
1	D	156	% 77% 17% ...
1	E	156	83% 12% ...

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Mol	Chain	Length	Quality of chain			
1	F	156		75%	16%	• • •
1	G	156		78%	14%	• • •
1	H	156		72%	15%	6% • •
1	I	156		75%	19%	• •
1	J	156		71%	21%	• • •
1	K	156		73%	19%	• • •
1	L	156		79%	13%	• • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14696 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NON-HEME IRON-CONTAINING FERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	B	151	Total	C	N	O	S	0	0	0
			1216	779	193	237	7			
1	C	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	D	150	Total	C	N	O	S	0	1	0
			1214	778	192	237	7			
1	E	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	F	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	G	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	H	149	Total	C	N	O	S	0	1	0
			1207	773	191	236	7			
1	I	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	J	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	K	149	Total	C	N	O	S	0	0	0
			1203	771	191	234	7			
1	L	152	Total	C	N	O	S	0	0	0
			1224	783	195	239	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	HIS	engineered mutation	UNP P80725
A	43	GLY	HIS	engineered mutation	UNP P80725
B	31	GLY	HIS	engineered mutation	UNP P80725
B	43	GLY	HIS	engineered mutation	UNP P80725
C	31	GLY	HIS	engineered mutation	UNP P80725

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Chain	Residue	Modelled	Actual	Comment	Reference
C	43	GLY	HIS	engineered mutation	UNP P80725
D	31	GLY	HIS	engineered mutation	UNP P80725
D	43	GLY	HIS	engineered mutation	UNP P80725
E	31	GLY	HIS	engineered mutation	UNP P80725
E	43	GLY	HIS	engineered mutation	UNP P80725
F	31	GLY	HIS	engineered mutation	UNP P80725
F	43	GLY	HIS	engineered mutation	UNP P80725
G	31	GLY	HIS	engineered mutation	UNP P80725
G	43	GLY	HIS	engineered mutation	UNP P80725
H	31	GLY	HIS	engineered mutation	UNP P80725
H	43	GLY	HIS	engineered mutation	UNP P80725
I	31	GLY	HIS	engineered mutation	UNP P80725
I	43	GLY	HIS	engineered mutation	UNP P80725
J	31	GLY	HIS	engineered mutation	UNP P80725
J	43	GLY	HIS	engineered mutation	UNP P80725
K	31	GLY	HIS	engineered mutation	UNP P80725
K	43	GLY	HIS	engineered mutation	UNP P80725
L	31	GLY	HIS	engineered mutation	UNP P80725
L	43	GLY	HIS	engineered mutation	UNP P80725

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	14	Total O 14 14	0	0
2	C	13	Total O 13 13	0	0
2	D	17	Total O 17 17	0	0
2	E	16	Total O 16 16	0	0
2	F	8	Total O 8 8	0	0
2	G	11	Total O 11 11	0	0
2	H	25	Total O 25 25	0	0
2	I	11	Total O 11 11	0	0
2	J	17	Total O 17 17	0	0

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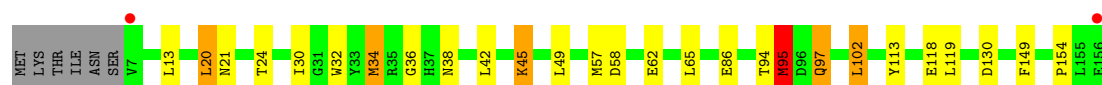
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	9	Total	O	0	0
			9	9		
2	L	14	Total	O	0	0
			14	14		

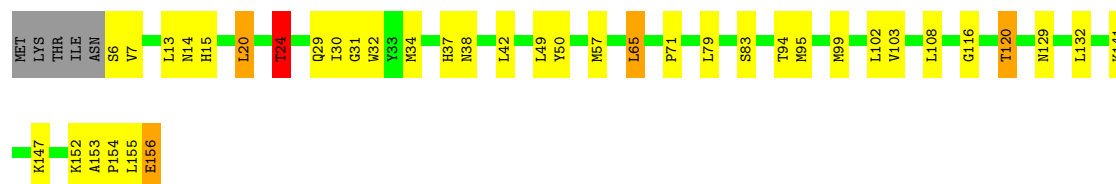
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

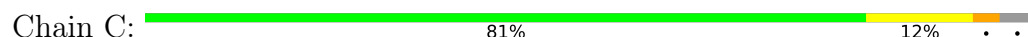
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



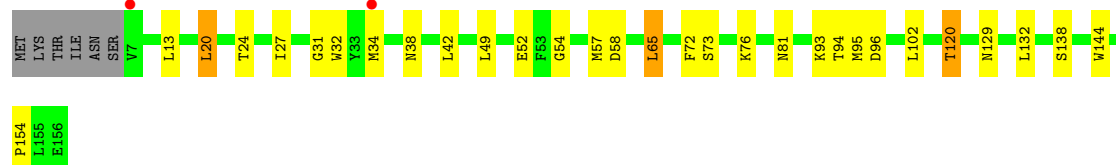
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



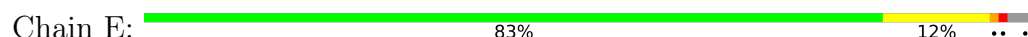
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



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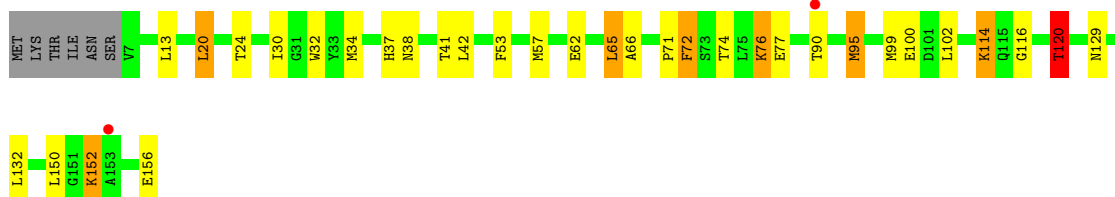
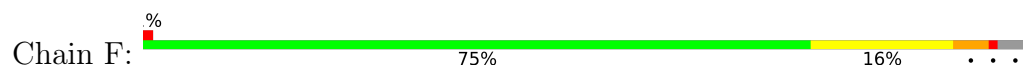


• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

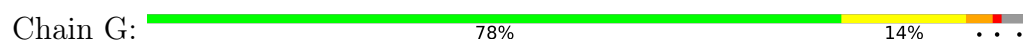




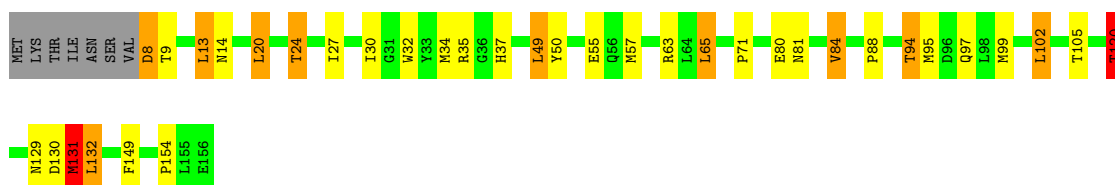
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



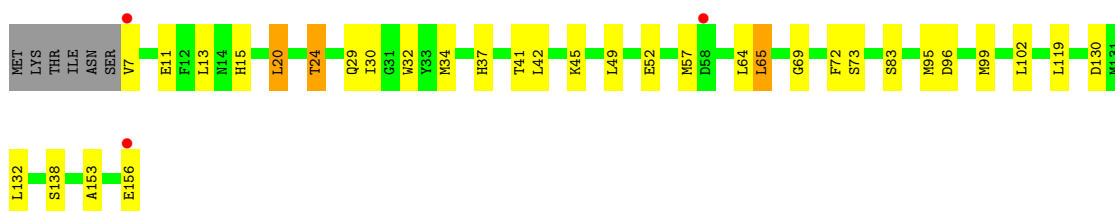
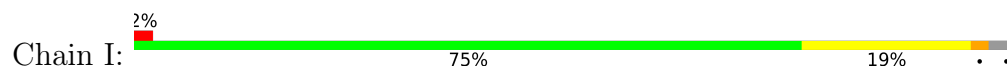
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



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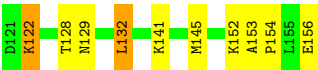


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

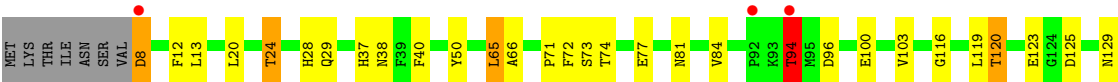


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

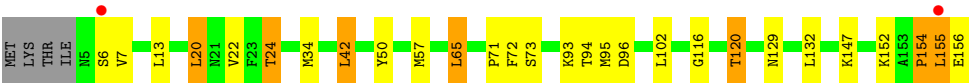
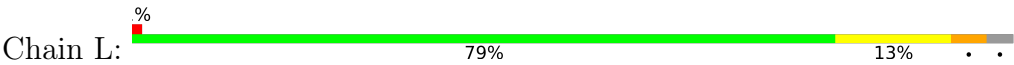




● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.62Å 132.21Å 168.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.60) 93.7 (30.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.207 , 0.252 0.208 , 0.207	Depositor DCC
R_{free} test set	2863 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14696	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	0/1235	1.50	3/1664 (0.2%)
1	B	1.03	0/1241	1.51	6/1672 (0.4%)
1	C	1.00	0/1235	1.48	0/1664
1	D	0.98	0/1243	1.44	2/1675 (0.1%)
1	E	0.97	0/1235	1.44	1/1664 (0.1%)
1	F	0.99	1/1235 (0.1%)	1.50	6/1664 (0.4%)
1	G	0.96	1/1235 (0.1%)	1.46	1/1664 (0.1%)
1	H	0.99	1/1236 (0.1%)	1.48	4/1665 (0.2%)
1	I	1.00	0/1235	1.50	3/1664 (0.2%)
1	J	0.99	0/1235	1.47	2/1664 (0.1%)
1	K	1.04	3/1228 (0.2%)	1.50	3/1654 (0.2%)
1	L	0.99	1/1249 (0.1%)	1.51	7/1683 (0.4%)
All	All	0.99	7/14842 (0.0%)	1.48	38/19997 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	1	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	84	VAL	CA-CB	6.47	1.61	1.54
1	G	94	THR	CA-CB	5.99	1.62	1.53
1	L	154	PRO	N-CD	-5.95	1.39	1.47
1	F	120	THR	CB-CG2	-5.77	1.33	1.52
1	K	120	THR	CB-CG2	-5.52	1.34	1.52
1	K	94	THR	CA-CB	5.17	1.61	1.53
1	K	84	VAL	CA-CB	5.11	1.59	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	VAL	N-CA-C	8.77	122.12	113.53
1	L	6	SER	N-CA-C	8.37	122.05	108.32
1	L	155	LEU	O-C-N	-8.14	110.80	122.36
1	L	155	LEU	CA-C-O	7.92	128.87	119.60
1	K	8	ASP	CB-CA-C	7.82	124.96	110.10
1	F	90	THR	CB-CA-C	7.71	122.76	111.65
1	H	8	ASP	CB-CA-C	7.58	124.51	110.10
1	H	131	MET	CB-CA-C	-6.30	100.73	110.81
1	A	95	MET	CA-C-N	6.24	128.55	120.44
1	A	95	MET	C-N-CA	6.24	128.55	120.44
1	L	7	VAL	N-CA-C	-6.14	99.62	108.53
1	A	34	MET	CG-SD-CE	-6.12	87.45	100.90
1	B	155	LEU	CA-C-N	6.08	132.65	121.70
1	B	155	LEU	C-N-CA	6.08	132.65	121.70
1	B	156	GLU	N-CA-CB	-5.96	100.37	110.50
1	J	41	THR	CB-CA-C	5.83	120.03	110.88
1	H	81	ASN	N-CA-C	5.67	121.23	113.97
1	F	72	PHE	N-CA-C	-5.58	102.14	110.23
1	L	155	LEU	N-CA-CB	5.58	118.70	110.33
1	I	41	THR	CB-CA-C	5.58	119.63	110.88
1	H	120	THR	CB-CA-C	5.56	121.94	110.31
1	I	72	PHE	N-CA-C	-5.54	102.20	110.23
1	D	72	PHE	N-CA-C	-5.48	102.28	110.23
1	K	72	PHE	N-CA-C	-5.48	102.28	110.23
1	L	155	LEU	N-CA-C	5.45	120.04	112.90
1	B	156	GLU	CA-CB-CG	5.42	124.93	114.10
1	L	72	PHE	N-CA-C	-5.35	102.48	110.23
1	F	120	THR	CB-CA-C	5.24	120.32	110.63
1	I	119	LEU	CA-CB-CG	5.22	134.57	116.30
1	G	41	THR	CB-CA-C	5.20	119.05	110.88
1	K	81	ASN	N-CA-C	5.14	120.20	113.88
1	F	53	PHE	CA-C-N	5.13	125.64	119.94
1	F	53	PHE	C-N-CA	5.13	125.64	119.94
1	B	24	THR	CB-CA-C	5.12	119.01	110.81
1	E	24	THR	CB-CA-C	5.12	119.28	110.79
1	D	81	ASN	N-CA-C	5.08	120.47	113.97
1	F	76	LYS	CB-CA-C	5.06	118.83	110.88
1	J	120	THR	CB-CA-C	5.06	120.38	110.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	K	8	ASP	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1210	0	1178	19	0
1	B	1216	0	1183	31	0
1	C	1210	0	1178	15	0
1	D	1214	0	1178	14	0
1	E	1210	0	1178	12	0
1	F	1210	0	1178	22	0
1	G	1210	0	1178	14	0
1	H	1207	0	1169	26	0
1	I	1210	0	1178	22	0
1	J	1210	0	1178	21	0
1	K	1203	0	1169	22	0
1	L	1224	0	1189	18	0
2	A	7	0	0	0	0
2	B	14	0	0	1	0
2	C	13	0	0	0	0
2	D	17	0	0	0	0
2	E	16	0	0	0	0
2	F	8	0	0	0	0
2	G	11	0	0	0	0
2	H	25	0	0	0	0
2	I	11	0	0	0	0
2	J	17	0	0	0	0
2	K	9	0	0	0	0
2	L	14	0	0	0	0
All	All	14696	0	14134	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLY:O	1:D:58[A]:ASP:OD2	1.91	0.87
1:I:153:ALA:HB3	1:I:156:GLU:HG2	1.63	0.80
1:L:147:LYS:NZ	1:L:156:GLU:C	2.41	0.78
1:J:38:ASN:HB3	1:J:42:LEU:HD23	1.69	0.73
1:L:147:LYS:HZ1	1:L:156:GLU:C	1.97	0.71
1:C:95:MET:HE3	1:C:95:MET:HA	1.74	0.69
1:G:116:GLY:O	1:G:120:THR:HB	1.92	0.68
1:B:38:ASN:HD21	1:J:37:HIS:HB3	1.59	0.68
1:F:95:MET:C	1:F:95:MET:SD	2.77	0.68
1:F:116:GLY:O	1:F:120:THR:HB	1.94	0.67
1:B:37:HIS:HB3	1:F:38:ASN:HD21	1.61	0.66
1:A:94:THR:H	1:A:97:GLN:HG3	1.60	0.65
1:D:120:THR:HG23	1:D:129:ASN:HB2	1.79	0.65
1:B:6:SER:HB3	2:B:2001:HOH:O	1.96	0.64
1:F:32:TRP:HB3	1:H:65:LEU:HD21	1.79	0.64
1:C:34:MET:HB3	1:C:95:MET:HE1	1.80	0.64
1:F:30:ILE:HG21	1:F:99:MET:HE1	1.79	0.64
1:F:150:LEU:O	1:F:152:LYS:HE3	1.97	0.64
1:B:156:GLU:CG	1:B:156:GLU:O	2.45	0.63
1:F:34:MET:SD	1:F:95:MET:HB2	2.38	0.63
1:B:20:LEU:HD23	1:B:57:MET:HA	1.80	0.63
1:J:120:THR:HG23	1:J:129:ASN:HB2	1.82	0.61
1:B:65:LEU:HD13	1:B:71:PRO:HD3	1.82	0.60
1:E:32:TRP:HB3	1:G:65:LEU:HD21	1.84	0.60
1:L:42:LEU:HD23	1:L:95:MET:SD	2.42	0.59
1:B:30:ILE:HG21	1:B:99:MET:HE1	1.83	0.59
1:K:24:THR:HG23	1:K:50:TYR:CE2	2.38	0.59
1:B:156:GLU:O	1:B:156:GLU:CD	2.46	0.58
1:D:38:ASN:HD21	1:I:37:HIS:HB3	1.67	0.58
1:B:116:GLY:O	1:B:120:THR:HB	2.03	0.58
1:L:94:THR:HG22	1:L:96:ASP:H	1.69	0.58
1:L:147:LYS:HZ3	1:L:156:GLU:C	2.11	0.58
1:F:76:LYS:HZ2	1:F:77:GLU:HG3	1.69	0.57
1:G:141:LYS:HG2	1:G:145:MET:HE2	1.87	0.57
1:H:120:THR:HG23	1:H:129:ASN:HB2	1.87	0.57
1:I:30:ILE:O	1:I:34:MET:HB2	2.04	0.57
1:A:36:GLY:O	1:H:149:PHE:HA	2.05	0.56
1:K:120:THR:HG23	1:K:125:ASP:HB3	1.87	0.56
1:B:153:ALA:O	1:B:156:GLU:HB2	2.05	0.56
1:E:38:ASN:HB3	1:E:42:LEU:HD23	1.87	0.56
1:A:94:THR:N	1:A:97:GLN:HG3	2.21	0.55
1:C:24:THR:HG23	1:C:50:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:HIS:HE1	1:J:83:SER:OG	1.89	0.55
1:B:34:MET:HB2	1:B:95:MET:SD	2.46	0.55
1:C:116:GLY:O	1:C:120:THR:HG22	2.07	0.54
1:L:24:THR:HG23	1:L:50:TYR:CE2	2.42	0.54
1:L:116:GLY:O	1:L:120:THR:HB	2.07	0.54
1:K:74:THR:OG1	1:K:77:GLU:HG3	2.07	0.54
1:E:34:MET:HB2	1:E:95:MET:HE1	1.90	0.54
1:H:34:MET:HB2	1:H:95:MET:HE1	1.90	0.54
1:J:141:LYS:HG2	1:J:145:MET:HE2	1.89	0.54
1:H:24:THR:HG23	1:H:50:TYR:CE2	2.43	0.53
1:C:34:MET:HE1	1:C:42:LEU:HB3	1.89	0.53
1:J:51:SER:O	1:J:55:GLU:HG2	2.07	0.53
1:H:30:ILE:HG21	1:H:99:MET:CE	2.39	0.53
1:H:37:HIS:HB3	1:K:38:ASN:OD1	2.09	0.52
1:B:30:ILE:HG21	1:B:99:MET:CE	2.38	0.52
1:H:24:THR:HG23	1:H:50:TYR:HE2	1.74	0.52
1:I:32:TRP:HB3	1:K:65:LEU:HD21	1.90	0.52
1:G:37:HIS:CE1	1:I:95:MET:HE1	2.45	0.52
1:J:153:ALA:HB3	1:J:156:GLU:HB2	1.92	0.52
1:F:74:THR:OG1	1:F:77:GLU:HG3	2.09	0.52
1:A:30:ILE:O	1:A:34:MET:HB2	2.10	0.52
1:A:32:TRP:HB3	1:C:65:LEU:HD21	1.92	0.52
1:I:30:ILE:HG21	1:I:99:MET:HE1	1.90	0.52
1:F:62:GLU:OE1	1:K:141:LYS:HE2	2.09	0.52
1:I:73:SER:HB2	1:K:29:GLN:HB2	1.92	0.52
1:G:120:THR:HG21	1:G:129:ASN:HA	1.92	0.52
1:E:29:GLN:HB2	1:G:73:SER:HB2	1.92	0.51
1:E:120:THR:HG21	1:E:129:ASN:HA	1.92	0.51
1:L:152:LYS:HB3	1:L:156:GLU:HG3	1.92	0.51
1:D:95:MET:SD	1:D:95:MET:C	2.94	0.51
1:G:94:THR:HG22	1:G:96:ASP:H	1.76	0.51
1:I:64:LEU:CD1	1:I:69:GLY:HA3	2.41	0.50
1:J:29:GLN:HB2	1:L:73:SER:HB2	1.93	0.50
1:D:31:GLY:HA2	1:D:34:MET:HE3	1.93	0.50
1:E:116:GLY:O	1:E:120:THR:HB	2.12	0.50
1:A:20:LEU:HD21	1:A:113:TYR:OH	2.11	0.50
1:D:20:LEU:HB3	1:D:57:MET:HB2	1.94	0.50
1:L:34:MET:HB2	1:L:95:MET:HE1	1.94	0.49
1:A:86:GLU:CD	1:C:74:THR:HB	2.37	0.49
1:K:8:ASP:HA	1:K:119:LEU:HD21	1.95	0.49
1:B:152:LYS:HD2	1:B:156:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ARG:HB3	1:K:151:GLY:HA2	1.94	0.49
1:I:20:LEU:O	1:I:24:THR:HB	2.13	0.49
1:B:65:LEU:HD13	1:B:71:PRO:CD	2.42	0.48
1:E:20:LEU:HB3	1:E:57:MET:HB2	1.94	0.48
1:B:120:THR:HG21	1:B:129:ASN:HA	1.94	0.48
1:H:30:ILE:HG21	1:H:99:MET:HE1	1.94	0.48
1:L:120:THR:HG23	1:L:129:ASN:HB2	1.95	0.48
1:A:65:LEU:O	1:E:154:PRO:HG2	2.13	0.48
1:C:65:LEU:O	1:H:154:PRO:HG2	2.12	0.48
1:A:154:PRO:HG2	1:I:65:LEU:O	2.14	0.48
1:L:120:THR:HG21	1:L:129:ASN:HA	1.96	0.48
1:G:120:THR:CG2	1:G:129:ASN:HA	2.44	0.48
1:A:95:MET:HE3	1:A:149:PHE:HE2	1.77	0.48
1:G:120:THR:HG23	1:G:129:ASN:HB2	1.95	0.48
1:E:120:THR:CG2	1:E:129:ASN:HA	2.45	0.47
1:H:27:ILE:HD13	1:H:49:LEU:HB3	1.96	0.47
1:D:120:THR:HG21	1:D:129:ASN:HA	1.97	0.47
1:J:118:GLU:HB3	1:J:122:LYS:HE2	1.95	0.47
1:G:147:LYS:HD2	1:G:152:LYS:HG3	1.96	0.47
1:A:49:LEU:HD21	1:A:102:LEU:HD21	1.96	0.47
1:F:65:LEU:O	1:K:154:PRO:HG2	2.15	0.47
1:I:30:ILE:HG21	1:I:99:MET:CE	2.44	0.47
1:I:52:GLU:OE2	1:I:138:SER:OG	2.32	0.47
1:I:57:MET:HE3	1:I:57:MET:HB3	1.76	0.47
1:C:34:MET:CB	1:C:95:MET:HE1	2.42	0.47
1:K:94:THR:HG22	1:K:96:ASP:H	1.79	0.46
1:D:52:GLU:OE2	1:D:138:SER:OG	2.29	0.46
1:H:65:LEU:HD13	1:H:71:PRO:CD	2.45	0.46
1:J:20:LEU:HB3	1:J:57:MET:HB2	1.97	0.46
1:K:12:PHE:CZ	1:K:116:GLY:HA3	2.50	0.46
1:C:153:ALA:HB3	1:C:156:GLU:HG3	1.97	0.46
1:F:114:LYS:HE3	1:F:114:LYS:O	2.15	0.46
1:A:20:LEU:HB3	1:A:57:MET:HB2	1.98	0.46
1:B:37:HIS:HB3	1:F:38:ASN:ND2	2.29	0.46
1:J:128:THR:O	1:J:132:LEU:HD22	2.16	0.46
1:I:15:HIS:HE1	1:I:83:SER:OG	2.00	0.45
1:B:32:TRP:HB3	1:D:65:LEU:HD21	1.97	0.45
1:I:29:GLN:HB2	1:K:73:SER:HB2	1.99	0.45
1:I:153:ALA:H	1:I:156:GLU:HG3	1.81	0.45
1:A:94:THR:H	1:A:97:GLN:CG	2.30	0.45
1:I:99:MET:HA	1:I:99:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:LEU:HD23	1:H:57:MET:HA	1.98	0.45
1:H:65:LEU:O	1:J:154:PRO:HG2	2.16	0.45
1:A:34:MET:HE1	1:A:95:MET:HG3	1.99	0.45
1:A:38:ASN:HD21	1:K:37:HIS:HB3	1.82	0.44
1:F:20:LEU:HD23	1:F:57:MET:HA	1.99	0.44
1:H:34:MET:HB2	1:H:95:MET:CE	2.47	0.44
1:I:34:MET:HE1	1:I:95:MET:HB2	2.00	0.44
1:I:153:ALA:HB3	1:I:156:GLU:CG	2.42	0.44
1:K:120:THR:HG21	1:K:129:ASN:N	2.32	0.44
1:B:154:PRO:HG3	1:L:65:LEU:O	2.17	0.44
1:D:27:ILE:HD13	1:D:49:LEU:HB3	1.99	0.44
1:D:154:PRO:HG2	1:K:65:LEU:O	2.16	0.44
1:L:154:PRO:O	1:L:155:LEU:HD23	2.17	0.44
1:G:24:THR:HG23	1:G:50:TYR:CE2	2.53	0.44
1:B:29:GLN:HB2	1:D:73:SER:HB2	1.98	0.44
1:G:34:MET:HE1	1:G:42:LEU:HB3	2.00	0.44
1:J:65:LEU:HD13	1:J:71:PRO:HD2	2.00	0.44
1:K:94:THR:HG22	1:K:96:ASP:N	2.32	0.44
1:F:72:PHE:HD2	1:F:77:GLU:OE2	2.01	0.44
1:B:15:HIS:HE1	1:B:83:SER:OG	2.01	0.43
1:B:152:LYS:HD2	1:B:156:GLU:CG	2.49	0.43
1:L:65:LEU:HD13	1:L:71:PRO:CD	2.48	0.43
1:B:24:THR:HG23	1:B:50:TYR:CE2	2.54	0.43
1:J:30:ILE:HG21	1:J:99:MET:CE	2.49	0.43
1:J:96:ASP:O	1:J:100:GLU:HG2	2.18	0.43
1:C:28:HIS:CE1	1:C:50:TYR:CE2	3.07	0.43
1:G:128:THR:HG22	1:G:132:LEU:HD22	2.00	0.43
1:L:20:LEU:HD23	1:L:57:MET:HA	2.00	0.43
1:L:120:THR:CG2	1:L:129:ASN:HA	2.49	0.43
1:B:99:MET:O	1:B:103:VAL:HG23	2.19	0.43
1:I:57:MET:HE1	1:K:28:HIS:CE1	2.53	0.43
1:J:75:LEU:HD22	1:L:22:VAL:HG22	2.01	0.43
1:D:144:TRP:HB2	1:K:66:ALA:HA	2.01	0.43
1:B:147:LYS:HE3	1:B:156:GLU:HB3	2.01	0.42
1:C:14:ASN:OD1	1:C:71:PRO:HA	2.18	0.42
1:C:76:LYS:O	1:C:80:GLU:HB2	2.19	0.42
1:B:108:LEU:HD23	1:B:108:LEU:C	2.44	0.42
1:B:14:ASN:OD1	1:B:71:PRO:HA	2.20	0.42
1:B:38:ASN:ND2	1:J:37:HIS:HB3	2.30	0.42
1:A:58:ASP:O	1:A:62:GLU:HG3	2.19	0.42
1:E:34:MET:HB2	1:E:95:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:ASN:OD1	1:H:71:PRO:HA	2.20	0.42
1:I:64:LEU:HD12	1:I:69:GLY:HA3	2.02	0.42
1:E:20:LEU:O	1:E:24:THR:HB	2.19	0.42
1:B:120:THR:HG23	1:B:129:ASN:HB2	2.00	0.42
1:F:37:HIS:HE1	1:J:96:ASP:OD2	2.02	0.42
1:E:73:SER:OG	1:G:29:GLN:HG3	2.20	0.42
1:J:20:LEU:HD23	1:J:57:MET:HA	2.01	0.42
1:A:34:MET:HE1	1:A:95:MET:CG	2.50	0.41
1:H:65:LEU:HD13	1:H:71:PRO:HD3	2.01	0.41
1:J:116:GLY:HA2	1:J:119:LEU:HD23	2.02	0.41
1:H:84:VAL:HG13	1:H:105:THR:HG23	2.02	0.41
1:B:31:GLY:HA2	1:B:34:MET:HE3	2.02	0.41
1:I:7:VAL:HB	1:I:11:GLU:HG3	2.01	0.41
1:F:76:LYS:NZ	1:H:88:PRO:HD3	2.35	0.41
1:F:156:GLU:CD	1:F:156:GLU:O	2.64	0.41
1:B:65:LEU:HD21	1:D:32:TRP:HB3	2.01	0.41
1:C:94:THR:HB	1:C:97:GLN:H	1.85	0.41
1:C:38:ASN:O	1:C:42:LEU:HB2	2.21	0.41
1:F:65:LEU:HD21	1:H:32:TRP:HB3	2.01	0.41
1:J:26:LYS:HE3	1:J:105:THR:OG1	2.20	0.41
1:A:21:ASN:OD1	1:A:57:MET:HE2	2.21	0.41
1:B:120:THR:CG2	1:B:129:ASN:HA	2.51	0.41
1:H:63:ARG:HG2	1:H:131:MET:HE2	2.03	0.41
1:K:65:LEU:HD13	1:K:71:PRO:HD3	2.01	0.40
1:F:65:LEU:HD13	1:F:71:PRO:CD	2.51	0.40
1:H:9:THR:HG22	1:H:13:LEU:HD22	2.03	0.40
1:A:45:LYS:HE3	1:K:40:PHE:CD2	2.56	0.40
1:F:66:ALA:HB1	1:K:140:ASP:HB3	2.03	0.40
1:H:131:MET:HE3	1:H:132:LEU:HD13	2.03	0.40
1:F:120:THR:HG22	1:F:129:ASN:HD22	1.84	0.40
1:H:94:THR:HG22	1:H:97:GLN:H	1.87	0.40
1:H:99:MET:SD	1:H:102:LEU:HD12	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	B	149/156 (96%)	148 (99%)	1 (1%)	0	100	100
1	C	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
1	D	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	E	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
1	F	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	G	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	H	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	I	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	J	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	K	147/156 (94%)	145 (99%)	2 (1%)	0	100	100
1	L	150/156 (96%)	148 (99%)	2 (1%)	0	100	100
All	All	1779/1872 (95%)	1757 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/137 (96%)	120 (92%)	11 (8%)	10	23
1	B	132/137 (96%)	120 (91%)	12 (9%)	9	19
1	C	131/137 (96%)	121 (92%)	10 (8%)	12	27
1	D	132/137 (96%)	120 (91%)	12 (9%)	9	19
1	E	131/137 (96%)	121 (92%)	10 (8%)	12	27
1	F	131/137 (96%)	118 (90%)	13 (10%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	131/137 (96%)	117 (89%)	14 (11%)	6	14
1	H	131/137 (96%)	117 (89%)	14 (11%)	6	14
1	I	131/137 (96%)	120 (92%)	11 (8%)	10	23
1	J	131/137 (96%)	116 (88%)	15 (12%)	5	11
1	K	130/137 (95%)	121 (93%)	9 (7%)	14	32
1	L	133/137 (97%)	124 (93%)	9 (7%)	14	32
All	All	1575/1644 (96%)	1435 (91%)	140 (9%)	9	20

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	20	LEU
1	A	24	THR
1	A	42	LEU
1	A	45	LYS
1	A	95	MET
1	A	97	GLN
1	A	102	LEU
1	A	118	GLU
1	A	119	LEU
1	A	130	ASP
1	B	13	LEU
1	B	20	LEU
1	B	24	THR
1	B	42	LEU
1	B	49	LEU
1	B	65	LEU
1	B	79	LEU
1	B	94	THR
1	B	102	LEU
1	B	120	THR
1	B	132	LEU
1	B	141	LYS
1	C	13	LEU
1	C	20	LEU
1	C	24	THR
1	C	42	LEU
1	C	45	LYS
1	C	65	LEU

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Mol	Chain	Res	Type
1	C	76	LYS
1	C	85	GLU
1	C	94	THR
1	C	132	LEU
1	D	13	LEU
1	D	20	LEU
1	D	24	THR
1	D	42	LEU
1	D	65	LEU
1	D	76	LYS
1	D	93	LYS
1	D	94	THR
1	D	96	ASP
1	D	102	LEU
1	D	120	THR
1	D	132	LEU
1	E	13	LEU
1	E	20	LEU
1	E	24	THR
1	E	55	GLU
1	E	65	LEU
1	E	94	THR
1	E	102	LEU
1	E	120	THR
1	E	121	ASP
1	E	132	LEU
1	F	13	LEU
1	F	20	LEU
1	F	24	THR
1	F	41	THR
1	F	42	LEU
1	F	65	LEU
1	F	95	MET
1	F	100	GLU
1	F	102	LEU
1	F	114	LYS
1	F	120	THR
1	F	132	LEU
1	F	152	LYS
1	G	7	VAL
1	G	13	LEU
1	G	20	LEU

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Mol	Chain	Res	Type
1	G	24	THR
1	G	42	LEU
1	G	55	GLU
1	G	65	LEU
1	G	94	THR
1	G	102	LEU
1	G	115	GLN
1	G	119	LEU
1	G	120	THR
1	G	130	ASP
1	G	132	LEU
1	H	8	ASP
1	H	13	LEU
1	H	20	LEU
1	H	24	THR
1	H	49	LEU
1	H	55	GLU
1	H	65	LEU
1	H	80	GLU
1	H	94	THR
1	H	102	LEU
1	H	120	THR
1	H	130	ASP
1	H	131	MET
1	H	132	LEU
1	I	13	LEU
1	I	20	LEU
1	I	24	THR
1	I	42	LEU
1	I	45	LYS
1	I	49	LEU
1	I	65	LEU
1	I	96	ASP
1	I	102	LEU
1	I	130	ASP
1	I	132	LEU
1	J	7	VAL
1	J	13	LEU
1	J	20	LEU
1	J	24	THR
1	J	41	THR
1	J	45	LYS

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Mol	Chain	Res	Type
1	J	65	LEU
1	J	102	LEU
1	J	114	LYS
1	J	118	GLU
1	J	119	LEU
1	J	120	THR
1	J	122	LYS
1	J	132	LEU
1	J	152	LYS
1	K	13	LEU
1	K	20	LEU
1	K	24	THR
1	K	65	LEU
1	K	94	THR
1	K	100	GLU
1	K	103	VAL
1	K	123	GLU
1	K	132	LEU
1	L	13	LEU
1	L	20	LEU
1	L	24	THR
1	L	42	LEU
1	L	65	LEU
1	L	93	LYS
1	L	102	LEU
1	L	120	THR
1	L	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	29	GLN
1	A	38	ASN
1	B	15	HIS
1	B	29	GLN
1	B	38	ASN
1	B	56	GLN
1	C	15	HIS
1	C	28	HIS
1	C	29	GLN
1	C	38	ASN

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Mol	Chain	Res	Type
1	C	81	ASN
1	D	15	HIS
1	D	38	ASN
1	E	15	HIS
1	E	29	GLN
1	E	81	ASN
1	F	15	HIS
1	F	28	HIS
1	F	37	HIS
1	F	38	ASN
1	F	129	ASN
1	G	15	HIS
1	G	37	HIS
1	H	37	HIS
1	H	38	ASN
1	I	15	HIS
1	I	38	ASN
1	J	15	HIS
1	J	129	ASN
1	K	15	HIS
1	K	28	HIS
1	K	56	GLN
1	K	81	ASN
1	K	115	GLN
1	K	129	ASN
1	L	15	HIS
1	L	28	HIS
1	L	81	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	150/156 (96%)	-0.31	2 (1%) 75 71	10, 18, 33, 41	0
1	B	151/156 (96%)	-0.34	0 100 100	12, 18, 33, 42	0
1	C	150/156 (96%)	-0.31	0 100 100	12, 18, 33, 39	0
1	D	150/156 (96%)	-0.30	2 (1%) 75 71	12, 18, 33, 39	1 (0%)
1	E	150/156 (96%)	-0.36	0 100 100	12, 18, 32, 41	0
1	F	150/156 (96%)	-0.31	2 (1%) 75 71	11, 18, 32, 43	0
1	G	150/156 (96%)	-0.34	0 100 100	10, 18, 32, 40	0
1	H	149/156 (95%)	-0.30	0 100 100	10, 18, 31, 40	1 (0%)
1	I	150/156 (96%)	-0.26	3 (2%) 65 60	10, 18, 32, 42	0
1	J	150/156 (96%)	-0.33	1 (0%) 84 82	10, 18, 32, 40	0
1	K	149/156 (95%)	-0.27	3 (2%) 65 60	11, 18, 31, 40	0
1	L	152/156 (97%)	-0.28	2 (1%) 75 71	11, 18, 34, 43	0
All	All	1801/1872 (96%)	-0.31	15 (0%) 82 80	10, 18, 33, 43	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	7	VAL	3.2
1	L	155	LEU	2.7
1	A	156	GLU	2.6
1	L	6	SER	2.6
1	I	156	GLU	2.6
1	K	94	THR	2.4
1	D	34	MET	2.4
1	K	8	ASP	2.4
1	D	7	VAL	2.4
1	A	7	VAL	2.3
1	I	58	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	92	PRO	2.3
1	F	153	ALA	2.2
1	F	90	THR	2.2
1	J	97	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.